Abstract

Prediction of grape compositional parameters using a Fourier transform near infrared instrument

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Introduction

The aim of this study was to investigate the potential of using a Fourier transform near infrared (FT-NIR) spectrophotometer attached with a transflectance probe to analyse colour, total soluble solids (TSS), dry matter (DM) and pH in red grape homogenate samples.

Materials and methods

Red grape homogenates ($n = 82$) sourced from three main grape varieties (Cabernet Sauvignon, Shiraz and Merlot) were analyzed using reference methods for color, TSS, DM and pH. A FT-NIR spectrophotometer, the ANTARIS® equipped with a transflectance probe (Thermo Fisher), able to generate spectra from 1100 to 2500 nm, was used. Spectral data were handled using The Unscrambler (v 9.5, CAMO, Norway) software to develop both calibration and prediction models for the chemical parameters analysed. Partial least squares regression (PLS) with internal full cross-validation was used to build the models.

Results and discussion

The accuracy of the models was evaluated using the coefficient of correlation in calibration (R^2) and the standard error of cross validation (*SECV*). Table 1 shows the R^2 and *SECV* on homogenised red grape samples for colour, DM, TSS and pH, respectively. Both TSS and DM were well predicted using the FT-NIR. Further studies are needed to improve the calibration accuracy and robustness for colour and pH in red grape homogenates.

Table 1. Cross-validation statistics to predict chemical compositional parameters in red grape homogenates ($n = 82$).

Constituents	R^2	*SECV*	*LV*	*RPD*
TSS (°Brix)	0.96	1.00	6	3.85
pH	0.74	0.13	8	1.70
Colour (mg g^{-1})*	0.64	0.18	10	1.80
DM (%)	0.85	2.30	13	2.10

TSS: total soluble solids, DM: dry matter, R^2: coefficient of determination in calibration; *SECV*: standard error of cross validation; *RPD*: *SD/SECV*; *LV*: latent variables.
*Expressed as the concentration of anthocyanins (malvidin-3-glucoside) in 1 g (fresh weight) homogenate.